CONTENTS

Theoretical study of N_{20} using semiempirical molecular orbital methods
C. Chen, L.-H. Lu and Y.-W. Yang (Taiwan, Republic of China) 1
Electronic structure of the polyatomic Zintl anion Sb_7^{3-}. A scattered-wave Xα study
C.A. Jolly and D.S. Marynick (Arlington, TX, USA) 9
On the comparison of results provided by different basis set quality criteria
T.L. Sordo and J.A. Sordo (Oviedo, Spain) 17
The molecular structure of the urea molecule: is the minimum energy structure planar?
R.J. Meier (Geleen, The Netherlands) and B. Coussens (Leuven-Heverlee, Belgium) 25
Effects of hydration on scale factors for ab initio force constants II
A.H. Lowrey (Washington, DC, USA) and R.W. Williams (Bethesda, MD, USA) 35
Effects of hydration on scale factors for ab initio force constants III: supermolecules
A.H. Lowrey (Washington, DC, USA) and R.W. Williams (Bethesda, MD, USA) 57
A theoretical study of the methanetriol decomposition mechanism
S. Böhm (Prague, Czechoslovakia), I. Senf and H.-D. Schädler (Halle-Wittenberg, Germany) and J. Kuthan (Prague, Czechoslovakia) 73
Scaled quantum mechanical force fields and interpretation of vibrational spectra of differently protonated adenine
J. Florián (Prague, Czechoslovakia) 83
Theoretical investigations of AlO_2
A.V. Nemukhin and J. Almlöf (Minneapolis, MN, USA) 101
Ab initio study on the Al_2O, Al_2O_2, Si_2O_2 and $AlSiO_2$ oxides and on the $LiAlO_2$ and $NaAlO_2$ molecules
L. Bencivenni (Rome, Italy), M. Pelino (L'Aquila, Italy) and F. Ramondo (Rome, Italy) 109
Ab initio study on the coordination structures of AsO_3^-, VO_3^- and CO_3^{2-} with alkali cations
F. Ramondo, L. Bencivenni, N. Sanna and S. Nunziante Cesaro (Rome, Italy) 121
Influence of fatty acid composition on the structure and stability of fatty acid complexes with vitamin E
I.L. Shamovsky, I.Yu. Yarovskaya, N.G. Khrapova and E.B. Burlakova (Moscow, USSR) 149
Ab initio study of Σ and Π electronic states of carbonyl radical cations
T. Nakano, K. Morihashi and O. Kikichi (Tsukuba, Japan) 161
Molecular orbital study of the electron donor–acceptor properties of the P atom in $Ni(PX_3)_4$ (X=H,F,Cl) complexes
M. Braga (Gothenburg, Sweden) 167
Conformational analysis of furan derivatives by semiempirical and experimental dipole moment determinations
P. Goya, A. Martínez, J. Plumet, C. Abradelo and I.H. Fuentes (Madrid, Spain), C. Cativiela and J.A. Mayoral (Zaragoza, Spain) 179
A quantum chemical study of the hydrogen bonding in a weakly bound SCO–HF complex
J. Sadlej (Lund, Sweden) 187
Ab initio study of the basis set dependence of the structural parameters, relative energies and fundamental frequencies of glyoxal
G.R. De Maré (Brussels, Belgium) 199
An ab initio investigation of some excited electronic states of the SiH_2^+ ion
J.-P. Gu and M.-B. Huang (Anhui, People's Republic of China, F. Kong (Beijing, People's Republic of China) and S.-H. Liu (Guangdong, People's Republic of China) 217
Structure energetics, and vibrational spectrum of H_2O–X^- (X=F,Cl) complexes
Z. Latajka (Wrocław, Poland) 225
Theoretical modelling of the electrophilic substitution mechanism in furan
J.R. Alvarez-Idaboy and L.A. Montero (Havana, Cuba) 243
Proton affinities of SNH and HSN. An ab initio study of the structures and stabilities of $(H_2NS)^+$
P. Redondo (Burgos, Spain) and A. Largo (Oviedo, Spain) 261

A quantum chemical study of the binding energies in the hydrates of Zn^{2+}, Cd^{2+} and Hg^{2+}
M.M. Probst (Innsbruck, Austria) 275
Singlet–triplet splittings and electron affinities of some substituted silylenes
J. Kalcher and A.F. Sax (Graz, Austria) 287
CI studies of four low-lying electronic states of the CNN radical
Z.-L. Cai, G.-H. Sha and C.-H. Zhang (Dalian, People's Republic of China) and M.-B. Huang (Hefei, People's Republic of China) 303
Moments of the electron-pair distribution function for first row diatomic molecules
M. Aguado, C. Sarasola, L. Dominguez and J.M. Ugalde (Euskadi, Spain) 311
An investigation of the electronic structure of the antitumor drug ellipticine and its derivatives. Part I. Geometrical AM1 study
S.O. Dantas, F.C. Lavarda, D.S. Galvão and B. Laks (Campinas, Brazil) 319
Many-body effects in the valence photoelectron spectra of the third row hydrides: a configuration interaction approach
A. Lisini, M. Brosolo, P. Decleva and G. Fronzoni (Trieste, Italy) 333
An AM1 study of conformational preference for the herbicide atrazine
W.B. De Almeida and P.J. O'Malley (Manchester, UK) 349
$(HCP)_2$ isomeric system: coexistence of T-shaped and linear structures
Z. Slanina (Mainz, Germany), W.B. De Almeida (Manchester, UK) and J.S. Craw (Sydney, NSW, Australia) 357
Many-body effects in the valence photoelectron spectra of the third row hydrides: a configuration interaction approach
A. Lisini, M. Brosolo, P. Decleva and G. Fronzoni (Trieste, Italy) 333
An AM1 study of conformational preference for the herbicide atrazine
W.B. De Almeida and P.J. O'Malley (Manchester, UK) 349
$(HCP)_2$ isomeric system: coexistence of T-shaped and linear structures
Z. Slanina (Mainz, Germany), W.B. De Almeida (Manchester, UK) and J.S. Craw (Sydney, NSW, Australia) 357
Valence bond representations for S_N2 reactions: one-electron delocalizations and electron-pair delocalizations
R.D. Harcourt (Parkville, Vic., Australia) 363

Short Communication
AM1 calculations of the proton affinity of azoles
V.K. Turchaninov and S.V. Yeroshchenko (Irkutsk, USSR) 371

Author Index 377

Subject Index 379